Project Proposal: Enzyme Kinetics and Michaelis-Menten Model Simulation

ESC113 Term Project - 2025 Even Semester

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1 Authors

- Prathmesh Thorat (241101)
- Kshitij Jain
- Rohan Upadhyay
- Falgun Dadhich
- Mayur Pachpute
- Madhur
- Thamesh Patra
- Priyanshu
- Krish Mundhra
- Dev Kushwaha

2 Introduction

Enzymes are important players in biochemical processes by speeding reaction rates. Familiarity of how substrate concentration and enzyme impact reaction velocity is central to chemical kinetics and biotechnology. Enzyme-catalyzed reactions are approximated using a mathematical model due to the Michaelis-Menten model. Solving the reaction kinetics mathematically manually is difficult. A computational strategy based on MATLAB can numerically solve differential equations and offer graphical understanding of reaction dynamics. In this project, enzyme kinetics shall be simulated according to the Michaelis-Menten model for the investigation of how substrate concentration, enzyme concentration, and conditions of the reaction affect reaction rates.

3 Objectives

- To develop a MATLAB-based GUI for simulating enzyme kinetics.
- To numerically solve and visualize the substrate consumption and product formation using first-order ordinary differential equations (ODEs).
- To analyze the effects of different parameters such as substrate concentration, enzyme concentration, and reaction rate constants on reaction speed.
- To plot reaction progress curves and analyze reaction rate dynamics

4 Methodology

The simulation will be developed using MATLAB and will involve the following steps:

4.1 Mathematical Model

The Michaelis-Menten equation, which describes the reaction rate, is given by:

$$v = \frac{V_{\max} S}{K_M + S} \tag{1}$$

where:

- v = rate of reaction
- S = substrate concentration
- $V_{\max} = k_2 E_0$ (maximum reaction velocity, depends on enzyme concentration)
- $K_M = \frac{k_{-1}+k_2}{k_1}$ (Michaelis constant, indicating enzyme efficiency)

The rate equations for substrate and product concentration are:

$$\frac{dS}{dt} = -\frac{V_{\max} S}{K_M + S} \tag{2}$$

$$\frac{dP}{dt} = \frac{V_{\max} S}{K_M + S} \tag{3}$$

4.2 MATLAB Implementation

1. **App Development**
   - Input fields for initial substrate concentration, enzyme concentration, and reaction time.
   - Buttons to start simulations and plot results.
2. **Numerical Computation**
   - Implement algorithms to solve ODE and IVP(initial value problems) problems
   - Compute and display reaction progress over time.

3. **Visualization & Analysis**

- Plot substrate concentration vs. time.
- Plot product concentration vs. time.
- Interactive analysis to observe changes when modifying enzyme or substrate concentrations.